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Preface to the Sixth Edition

Since the fifth edition was published in 1996, a number of new developments have been made in the field of infrared and Raman spectra of inorganic and coordination compounds. The sixth edition is intended to emphasize new important developments as well as to catch up with the ever-increasing new literature. Major changes are described below.

Part A. Chapter 1 ("Theory of Normal Vibrations") includes two new sections. Section 1.24 explains the procedure for calculating vibrational frequencies on the basis of density functional theory (DFT). The DFT method is currently used almost routinely to determine molecular structures and to calculate vibrational parameters. Section 1.26 describes new developments in matrix condensation techniques. More recently, a large number of novel inorganic and coordination compounds have been prepared by using this technique, and their structures have been determined and vibrational assignments have been made on the basis of results of DFT calculations. Chapter 2 ("Applications in Inorganic Chemistry") has been updated extensively, resulting in a total number of references of over 1800. In particular, sections on trigonal X_3 - and tetrahedral X_4 -type molecules have been added as Secs. 2.3 and 2.5, respectively. In Sec. 2.3, the rotational–vibrational spectrum of the octahedral UF_6 molecule is shown to demonstrate how an extremely small metal isotope shift by $^{235}\text{U}/^{238}\text{U}$ substitution (only 0.0040cm^{-1}) can be measured. Section 2.14 ("Compounds of Carbon") has been expanded to show significant applications of vibrational spectroscopy to the structural determination of fullerenes, endohedral fullerenes, and carbon nanotubes. Vibrational data on a number of novel inorganic compounds prepared most recently have been added throughout Chapter 2.

Part B. Chapter 1 ("Applications in Coordination Chemistry") contains two new Sections: Sec. 1.4 ("Metallochlorins, Chlorophylls, and Metallophthalocyanines")